

**J. Gmehling
U. Onken**

VAPOR-LIQUID EQUILIBRIUM DATA COLLECTION

**Aqueous Systems
Supplement 3
Br₂ – C₄H₁₀O**



Chemistry Data Series

**Vol. I, Part 1c
(in conjunction with Part 1d)**

**Published by DECHEMA
Gesellschaft für Chemische Technik und Biotechnologie e.V.**

Executive Editor: Gerhard Kreysa

Bibliographic information published by Die Deutsche Bibliothek

Die Deutsche Bibliothek lists this publication in the Deutsche Nationalbibliographie; detailed bibliographic data is available on the Internet at <http://dnb.ddb.de>

ISBN: 3-89746-053-X

© DECHEMA Deutsche Gesellschaft für Chemisches Apparatewesen,
Chemische Technik und Biotechnologie e. V.
Postfach 15 01 04, D-60061 Frankfurt am Main, Germany, 2003

Dieses Werk ist urheberrechtlich geschützt. Alle Rechte, auch die der Übersetzung, des Nachdrucks und der Vervielfältigung des Buches oder Teilen daraus sind vorbehalten.

Kein Teil des Werkes darf ohne schriftliche Genehmigung der DECHEMA in irgendeiner Form (Fotokopie, Mikrofilm oder einem anderen Verfahren), auch nicht für Zwecke der Unterrichtsgestaltung, reproduziert oder unter Verwendung elektronischer Systeme verarbeitet, vervielfältigt oder verbreitet werden.

Die Herausgeber übernehmen für die Richtigkeit und Vollständigkeit der publizierten Daten keinerlei Gewährleistung.

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, including those of translation, reprinting, reproduction by photocopying machine or similar means.

No part of this work may be reproduced, processed or distributed in any form, not even for teaching purposes – by photocopying, microfilm or other processes, or implemented in electronic information storage and retrieval systems – without the written permission of the publishers.

The publishers accept no liability for the accuracy and completeness of the published data.

This volume of the Chemistry Data Series was printed using acid-free paper.

Technical Production: Media Process Management, Mainz, www.digitalagentur-mpm.de

Vapor-Liquid Equilibrium Data Collection

1 c

Aqueous Systems

Supplement 3

Br₂ – C₄H₁₀O

Tables and diagrams of data for binary and multicomponent mixtures up to moderate pressures. Constants of correlation equations for computer use.

J. Gmehling, U. Onken

Technische Chemie
Universität Oldenburg

1 c

**Aqueous Systems
(Supplement 3)**

Br₂ - C₄H₁₀O

SUBJECTS OF VOLUME I

The subjects of Volume I in the Chemistry Data Series (CDS) are:

Subtitle	Vol. I, Part
Aqueous Systems	1 1a 1b 1c 1d
Organic Hydroxy Compounds	
Alcohols	2a
Alcohols and Phenols	2b 2c 2d 2e 2f
Aldehydes, Ketones, Ethers	3/4
Aldehydes	3a
Ketones	3b
Ethers	4a 4b
Carboxylic Acids, Anhydrides, Esters	5
Carboxylic Acids, Anhydrides	5a
Esters	5b
Aliphatic Hydrocarbons C ₄ -C ₆	6a
Aliphatic Hydrocarbons C ₇ -C ₁₈	6b 6c
Aliphatic Hydrocarbons C ₄ -C ₃₀	6d/e
Aromatic Hydrocarbons	7 7a 7/b
Halogen, Nitrogen, Sulfur and other compounds	8 8a

A substance index to Volume I on CD-ROM is available from the DECHEMA e.V. and its agents.

AUTHORS' PREFACE

With this publication we continue the series of supplements of our Vapor-Liquid Equilibrium Data Collection (Part 1) for aqueous systems. Due to the large amount of data the collection will be published as two books, to be sold as one publication. The indexes are to be found at the end of Volumes I 1c and 1d.

The data in this book are taken from the Dortmund Data Bank. The Dortmund Data Bank covers a wide range of properties in addition to VLE, LLE, h^E , γ^∞ , azeotropic data, e.g. gas solubilities, solid-liquid equilibria and the largest collection of pure component properties. The Dortmund Data Bank is also available in electronic form. The electronic version can be obtained from DDBST GmbH, Oldenburg (www.ddbst.de), Germany, DECHEMA e.V., Frankfurt am Main, Germany or FIZ Chemie, Berlin, Germany. DDBST can also supply a software package designed to process the data and to use them efficiently for process simulation. Online versions of the data base as DETHERM are hosted by STN International (Columbus, Ohio, USA, Karlsruhe, Germany and Tokyo, Japan) and DECHEMA e.V. (via the Internet as DETHERM... on the WEB). The publication of this collection would not have been possible without the cooperation and labors of all our colleagues at DDBST GmbH, in particular: J. Menke, J. Krafczyk and Dr. J. Ahlers.

In this work parameters have often not been published, because experimental data is only available for a limited concentration range, often caused by a large miscibility gap. Binary parameters have not been fitted for systems with strong electrolytes, e.g. sulfuric acid, hydrochloric acid, nitric acid or where chemical reactions, e.g. in systems containing formaldehyde need to be taken into account.

The role of the editorial team in scientific book production is often undervalued. We however recognize the worth of the endeavors of Dr. R. Sass and Dr. N. Forsyth with other members of the Information System and Data Base Department at DECHEMA e.V. and would like to express our gratitude for their rapid and efficient transformation of a collection of pages of data into a finished book.

Oldenburg, November 2003

J. Gmehling

U. Onken

EXECUTIVE EDITOR'S PREFACE

The aim of DECHEMA e.V., The Society for Chemical Technology and Biotechnology when it was founded in 1926 was to improve cooperation between chemist and engineer). As the importance of mathematical modelling, computer simulation and optimisation became apparent in the mid-nineteen-seventies, this ideal resulted in the production and publication of collections of basic thermophysical data in both electronic and book form. This is not data that could have easily found a publisher outside the engineering societies, because of its sheer volume and limited circle of interest. By its sponsoring and publication of the DECHEMA Chemistry Data Series DECHEMA e.V. has been associated with these endeavours for over a quarter of a century. Much of the original work to determine the values obtained was financed by the German Ministry of Research.

It is to be hoped that publication of this data collection by DECHEMA e.V. in the DECHEMA Chemistry Data Series will inspire other authors to consider publishing their collections of thermophysical data. DECHEMA e.V. is always pleased to assist colleagues from the thermophysical data community in preparing their results, their studies, their collections and their assessments for publication. DECHEMA e.V. is always prepared to enlarge the scope of the DECHEMA Chemistry Data Series and is thus pleased to hear from readers, designers, scientists and engineers of areas where thermophysical data is not available or scarce. We hope that the end user finds the data of utility and of interest.

Frankfurt am Main, November 2003

Gerhard Kreysa

CONTENTS
Vol. I, Part 1c

In Part 1c:

Subjects of Chemistry Data Series Vol. I	VI
Author's Preface	VII
Executive Editor's Preface	VIII
Contents Vol. I, Part 1c	IX
Guide to Tables	XI
References	XXIII

Data Tables

Binary Systems	1
Appendix A: Pure Component Parameters	623
Appendix B: Dimerization Constants of Carboxylic Acids	637
Formula Index of Binary Systems	639
Alphabetical Index of Binary Systems	643

Part 1c contains pages I-XXIII and 1-646

R = Recommended Values

Br ₂	Bromine	H ₂ O	Water	1
HBr	Hydrogen Bromide	H ₂ O	Water	2
HCl	Hydrogen Chloride	H ₂ O	Water	3
HNO ₃	Nitric Acid	H ₂ O	Water	4–14
H ₂ O ₄ S	Sulfuric Acid	H ₂ O	Water	15–23
H ₃ O ₄ P	Phosphoric Acid	H ₂ O	Water	24–30
H ₄ N ₂	Hydrazine	H ₂ O	Water	31–34
CClN	Cyanogen Chloride	H ₂ O	Water	35
CH ₂ Cl ₂	Dichloromethane	H ₂ O	Water	36
CH ₂ O	Formaldehyde	H ₂ O	Water	37–40
CH ₂ O ₂	Formic Acid	H ₂ O	Water	41–50, 51 R
CH ₃ NO	Formamide	H ₂ O	Water	52
CH ₃ NO ₂	Nitromethane	H ₂ O	Water	53–54
CH ₄ N ₂ O	Carbonyl Diamide <Urea>	H ₂ O	Water	55–56
CH ₄ O	Methanol	H ₂ O	Water	57–100, 101 R
CH ₄ S	Methanethiol	H ₂ O	Water	103
CH ₆ N ₂	Methylhydrazine	H ₂ O	Water	104–107
C ₂ HCl ₃ O ₂	Trichloroacetic Acid	H ₂ O	Water	108–109
C ₂ H ₂ Cl ₂ O ₂	Dichloroacetic Acid	H ₂ O	Water	110
C ₂ H ₃ ClO ₂	Chloroacetic Acid	H ₂ O	Water	111–113
C ₂ H ₃ F ₃ O	2,2,2-Trifluoroethanol	H ₂ O	Water	114–121
C ₂ H ₃ N	Acetonitrile	H ₂ O	Water	122–129, 130 R
C ₂ H ₄ Cl ₂	1,2-Dichlorethane	H ₂ O	Water	131–132
C ₂ H ₄ O	Acetaldehyde	H ₂ O	Water	133–137
	Ethylene Oxide	H ₂ O	Water	138

C ₂ H ₄ O ₂	Acetic Acid	H ₂ O	Water	139–166, 167 R
	Methyl Formate	H ₂ O	Water	170–171
C ₂ H ₅ Br	Ethyl Bromide	H ₂ O	Water	172
C ₂ H ₅ NO	n-Methylformamide	H ₂ O	Water	173–174
C ₂ H ₆ O	Ethanol	H ₂ O	Water	175–253, 254 R
C ₂ H ₆ OS	Dimethyl Sulfoxide	H ₂ O	Water	257–274
C ₂ H ₆ O ₂	1,2-Ethanediol (Ethylene Glycol)	H ₂ O	Water	275–285, 286 R
C ₂ H ₆ S	Ethanethiol	H ₂ O	Water	287
C ₂ H ₇ N	Dimethylamine	H ₂ O	Water	288
	Ethylamine	H ₂ O	Water	289
C ₂ H ₇ NO	Monoethanolamine	H ₂ O	Water	290–295, 296 R
C ₂ H ₈ N ₂	1,1-Dimethylhydrazine	H ₂ O	Water	297–299
C ₃ H ₂ F ₆ O	1,1,1,3,3,3-Hexafluoro-2-Propanol	H ₂ O	Water	300–301
C ₃ H ₃ N	Acrylonitrile	H ₂ O	Water	302–304
C ₃ H ₄ O	Acrolein	H ₂ O	Water	305–306
C ₃ H ₅ ClO	Epichlorohydrin	H ₂ O	Water	307
C ₃ H ₅ N	Propionitrile	H ₂ O	Water	308
C ₃ H ₆ O	Acetone	H ₂ O	Water	309–345, 346 R
	Allyl Alcohol	H ₂ O	Water	348–355, 356 R
	Propanal	H ₂ O	Water	357–359
C ₃ H ₆ O ₂	1,3-Dioxolane	H ₂ O	Water	360–368, 369 R
	2,3-Epoxy-1-Propanol	H ₂ O	Water	370–371
	Ethyl Formate	H ₂ O	Water	372–375

	Methyl Acetate	H ₂ O	Water	376
	Propionic Acid	H ₂ O	Water	377–380
C ₃ H ₆ O ₃	1,3,5-Trioxane	H ₂ O	Water	381–387
C ₃ H ₇ NO	n,n-Dimethylformamide (DMF)	H ₂ O	Water	388–401
	n-Methylacetamide	H ₂ O	Water	402–404
C ₃ H ₈ O	1-Propanol	H ₂ O	Water	405–424, 425 R
	2-Propanol	H ₂ O	Water	427–444, 445 R
C ₃ H ₈ O ₂	Dimethoxymethane	H ₂ O	Water	448–456
	2-Methoxy-Ethanol	H ₂ O	Water	457–466
	1,2-Propanediol	H ₂ O	Water	467–472, 473 R
	1,3-Propanediol	H ₂ O	Water	474–477
C ₃ H ₈ O ₃	Glycerol	H ₂ O	Water	478–484
C ₃ H ₈ S	1-Propanethiol	H ₂ O	Water	485
C ₃ H ₉ N	Trimethylamine	H ₂ O	Water	486–489
C ₃ H ₉ NO	3-Amino-1-Propanol	H ₂ O	Water	490–497
C ₃ H ₁₀ N ₂	Propylenediamine	H ₂ O	Water	498
C ₄ H ₅ N	Pyrrole	H ₂ O	Water	499–500
C ₄ H ₆ O	Crotonaldehyde	H ₂ O	Water	501–504
C ₄ H ₆ O ₂	2-Butyne-1,4-diol	H ₂ O	Water	505–512
	Gamma-Butyrolactone	H ₂ O	Water	513–517
	Methacrylic Acid	H ₂ O	Water	518–521
	Vinyl Acetate	H ₂ O	Water	522
C ₄ H ₇ NO	2-Methyl Propenoic Acid Amide (Methacrylamide)	H ₂ O	Water	523
C ₄ H ₈ O	2-Butanone	H ₂ O	Water	524–529
	1-Buten-3-ol	H ₂ O	Water	530
	Butyraldehyde	H ₂ O	Water	531–533

	2-Methylpropanal	H ₂ O	Water	534–535
	Tetrahydrofuran	H ₂ O	Water	536–538
C ₄ H ₈ O ₂	Butyric Acid	H ₂ O	Water	539
	1,4-Dioxane	H ₂ O	Water	540–549
	Ethyl Acetate	H ₂ O	Water	550–554
	2-Methyl-1,3-Dioxolane	H ₂ O	Water	555–558
	Methyl Propionate	H ₂ O	Water	559–561
C ₄ H ₈ O ₂ S	Sulfolane	H ₂ O	Water	562–563
C ₄ H ₈ O ₃	Methyl Methoxyacetate	H ₂ O	Water	564
C ₄ H ₉ N	Pyrrolidine	H ₂ O	Water	565–566
C ₄ H ₉ NO	n,n-Dimethylacetamide	H ₂ O	Water	567
	Morpholine	H ₂ O	Water	568–569
C ₄ H ₁₀ N ₂	Piperazine	H ₂ O	Water	570
C ₄ H ₁₀ O	1-Butanol	H ₂ O	Water	571–580, 581 R
	2-Butanol	H ₂ O	Water	582–591, 592 R
	2-Methyl-1-Propanol	H ₂ O	Water	593–598
	Tert-Butanol	H ₂ O	Water	599–621

R = Recommended Values

Acetaldehyde	C ₂ H ₄ O	Water	H ₂ O	133–137
Acetic Acid	C ₂ H ₄ O ₂	Water	H ₂ O	139–166, 167 R
Acetone	C ₃ H ₆ O	Water	H ₂ O	309–345, 346 R
Acetonitrile	C ₂ H ₃ N	Water	H ₂ O	122–129, 130 R
Acrolein	C ₃ H ₄ O	Water	H ₂ O	305–306
Acrylonitrile	C ₃ H ₃ N	Water	H ₂ O	302–304
Allyl Alcohol	C ₃ H ₆ O	Water	H ₂ O	348–355, 356 R
3-Amino-1-Propanol	C ₃ H ₉ NO	Water	H ₂ O	490–497
Bromine	Br ₂	Water	H ₂ O	1
1-Butanol	C ₄ H ₁₀ O	Water	H ₂ O	571–580, 581 R
2-Butanol	C ₄ H ₁₀ O	Water	H ₂ O	582–591, 592 R
Tert-Butanol	C ₄ H ₁₀ O	Water	H ₂ O	599–621
2-Butanone	C ₄ H ₈ O	Water	H ₂ O	524–529
1-Buten-3-ol	C ₄ H ₈ O	Water	H ₂ O	530
2-Butyne-1,4-diol	C ₄ H ₆ O ₂	Water	H ₂ O	505–512
Butyraldehyde	C ₄ H ₈ O	Water	H ₂ O	531–533
Butyric Acid	C ₄ H ₈ O ₂	Water	H ₂ O	539
Gamma-Butyrolactone	C ₄ H ₆ O ₂	Water	H ₂ O	513–517
Carbonyl Diamide	CH ₄ N ₂ O	Water	H ₂ O	55–56
Chloroacetic Acid	C ₂ H ₃ ClO ₂	Water	H ₂ O	111–113
Crotonaldehyde	C ₄ H ₆ O	Water	H ₂ O	501–504
Cyanogen Chloride	CClN	Water	H ₂ O	35
1,2-Dichlorethane	C ₂ H ₄ Cl ₂	Water	H ₂ O	131–132
Dichloroacetic Acid	C ₂ H ₂ Cl ₂ O ₂	Water	H ₂ O	110
Dichloromethane	CH ₂ Cl ₂	Water	H ₂ O	36

Dimethoxymethane	$C_3H_8O_2$	Water	H_2O	448–456
Dimethyl Sulfoxide	C_2H_6OS	Water	H_2O	257–274
n,n-Dimethylacetamide	C_4H_8NO	Water	H_2O	567
Dimethylamine	C_2H_7N	Water	H_2O	288
n,n-Dimethylformamide (DMF)	C_3H_7NO	Water	H_2O	388–401
1,1-Dimethylhydrazine	$C_2H_8N_2$	Water	H_2O	297–299
1,4-Dioxane	$C_4H_8O_2$	Water	H_2O	540–549
1,3-Dioxolane	$C_3H_6O_2$	Water	H_2O	360–368, 369 R
Epichlorohydrin	C_3H_5ClO	Water	H_2O	307
2,3-Epoxy-1-Propanol	$C_3H_6O_2$	Water	H_2O	370–371
1,2-Ethanediol (Ethylene Glycol)	$C_2H_6O_2$	Water	H_2O	275–285, 286 R
Ethanethiol	C_2H_6S	Water	H_2O	287
Ethanol	C_2H_6O	Water	H_2O	175–253, 254 R
Ethyl Acetate	$C_4H_8O_2$	Water	H_2O	550–554
Ethyl Bromide	C_2H_5Br	Water	H_2O	172
Ethyl Formate	$C_3H_6O_2$	Water	H_2O	372–375
Ethylamine	C_2H_7N	Water	H_2O	289
Ethylene Oxide	C_2H_4O	Water	H_2O	138
Formaldehyde	CH_2O	Water	H_2O	37–40
Formamide	CH_3NO	Water	H_2O	52
Formic Acid	CH_2O_2	Water	H_2O	41–50, 51 R
Glycerol	$C_3H_8O_3$	Water	H_2O	478–484
1,1,1,3,3,3-Hexafluoro-2-Propanol	$C_3H_2F_6O$	Water	H_2O	300–301

Hydrazine	H ₄ N ₂	Water	H ₂ O	31–34
Hydrogen Bromide	HBr	Water	H ₂ O	2
Hydrogen Chloride	HCl	Water	H ₂ O	3
Methacrylic Acid	C ₄ H ₆ O ₂	Water	H ₂ O	518–521
Methanethiol	CH ₄ S	Water	H ₂ O	103
Methanol	CH ₄ O	Water	H ₂ O	57–101, 102 R
2-Methoxy-Ethanol	C ₃ H ₈ O ₂	Water	H ₂ O	457–466
Methyl Acetate	C ₃ H ₆ O ₂	Water	H ₂ O	376
Methyl Formate	C ₂ H ₄ O ₂	Water	H ₂ O	170–171
Methyl Methoxyacetate	C ₄ H ₈ O ₃	Water	H ₂ O	564
2-Methyl Propenoic Acid Amide (Methacrylamide)	C ₄ H ₇ NO	Water	H ₂ O	523
Methyl Propionate	C ₄ H ₈ O ₂	Water	H ₂ O	559–561
n-Methylacetamide	C ₃ H ₇ NO	Water	H ₂ O	402–404
2-Methyl-1,3-Dioxolane	C ₄ H ₈ O ₂	Water	H ₂ O	555–558
n-Methylformamide	C ₂ H ₅ NO	Water	H ₂ O	173–174
Methylhydrazine	CH ₆ N ₂	Water	H ₂ O	104–107
2-Methylpropanal	C ₄ H ₈ O	Water	H ₂ O	534–535
2-Methyl-1-Propanol	C ₄ H ₁₀ O	Water	H ₂ O	593–598
Monoethanolamine	C ₂ H ₇ NO	Water	H ₂ O	290–295, 296 R
Morpholine	C ₄ H ₉ NO	Water	H ₂ O	568–569
Nitric Acid	HNO ₃	Water	H ₂ O	4–14
Nitromethane	CH ₃ NO ₂	Water	H ₂ O	53–54
Phosphoric Acid	H ₃ O ₄ P	Water	H ₂ O	24–30
Piperazine	C ₄ H ₁₀ N ₂	Water	H ₂ O	570

Propanal	C_3H_6O	Water	H_2O	357–359
1,2-Propanediol	$C_3H_8O_2$	Water	H_2O	467–472, 473 R
1,3-Propanediol	$C_3H_8O_2$	Water	H_2O	474–477
1-Propanethiol	C_3H_8S	Water	H_2O	485
1-Propanol	C_3H_8O	Water	H_2O	405–424, 425 R
2-Propanol	C_3H_8O	Water	H_2O	427–444, 445 R
Propionic Acid	$C_3H_6O_2$	Water	H_2O	377–380
Propionitrile	C_3H_5N	Water	H_2O	308
Propylenediamine	$C_3H_{10}N_2$	Water	H_2O	498
Pyrrole	C_4H_5N	Water	H_2O	499–500
Pyrrolidine	C_4H_9N	Water	H_2O	565–566
Sulfolane	$C_4H_8O_2S$	Water	H_2O	562–563
Sulfuric Acid	H_2O_4S	Water	H_2O	15–23
Tetrahydrofuran	C_4H_8O	Water	H_2O	536–538
Trichloroacetic Acid	$C_2HCl_3O_2$	Water	H_2O	108–109
2,2,2-Trifluoroethanol	$C_2H_3F_3O$	Water	H_2O	114–121
Trimethylamine	C_3H_9N	Water	H_2O	486–489
1,3,5-Trioxane	$C_3H_6O_3$	Water	H_2O	381–387
Urea	CH_4N_2O	Water	H_2O	55–56
Vinyl Acetate	$C_4H_6O_2$	Water	H_2O	522